

Premixer Design for High Hydrogen Fuels

Technical Progress Report

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ABSTRACT

This 18-month project translates DLN technology to the unique properties of high hydrogen content IGCC fuels, and will yield a design in preparation for a future testing and validation phase. Fundamental flame characterization, mixing, and flame property measurement experiments will be conducted to tailor computational design tools and criteria to create a framework for predicting nozzle operability (e.g., flame stabilization, emissions, resistance to flashback/flame-holding and auto-ignition). This framework is then used to establish, rank, and evaluate potential solutions to the operability challenges of IGCC combustion. The leading contenders are then studied and developed with the most promising concepts evaluated via computational fluid dynamics (CFD) modeling and using the design rules generated by the fundamental experiments as well as using GE's combustion design tools and practices. Finally, this project will scope the necessary steps required to carry the design through mechanical and durability review, testing, and validation, towards full demonstration of this revolutionary technology.

This project is being carried out in three linked tasks with the following results to date.

1. Develop conceptual designs of premixer and down-select the promising options.

This task defined the "gap" between existing design capabilities and the targeted range of IGCC fuel compositions and evaluated the current capability of DLN pre-mixer designs when operated at similar conditions. Two concepts 1) swirl based and 2) multiple point lean direct injection based premixers were selected via a QFD from 13 potential design concepts. This task was completed and reported on in the previous semi-annual report.

2. Carry out CFD on chosen options (1 or 2) to evaluate operability risks.

This task developed the leading options down-selected in Task 1. Both a GE15 swozzle based premixer and a lean direct injection concept were examined by performing a detailed CFD study wherein the aerodynamics of the design, together with the chemical kinetics of the combustion process was analyzed to evaluate the performance of the different concepts. Detailed 1-D analysis was performed to provide 1-step NOx and 1-step combustion models that could be utilized in CFD to provide more accurate estimates of NOx for more complicated combustion designs The swozzle results identified potential problems with flame holding, flashback and with adequate mixing. Flame holding issues were further evaluated with laboratory testing to determine under what conditions a jet in cross flow would flame hold. Additional CFD analysis was also performed on fuel injection from a peg to simulate fuel injection off a vane's trailing edge. This task was concluded with a Conceptual Design Review of the two selected design concepts.

3. Optimize design and re-evaluate operability risks.

This task extended the analysis of LDI concepts and increased understanding of the optimal design configuration. Designs were selected for subscale combustion laboratory testing. As experimental results from the tests become available, the CFD models will be further developed to improve accuracy. Different swirler designs were also evaluated and the most promising selected for further evaluation. This task is still in progress.

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Introduction

Premixer Design for High Hydrogen Fuels

A. Objective:

This study will develop combustion technology that will enable fuel flexible gas turbines that are capable of operating on coal derived synthetic gas to achieve NOx emissions corrected to 15% Oxygen by volume of 2 ppmvd or less at the exit of the gas turbine. Today, the combustion of Integrated Gasification Combined Cycle (IGCC) fuels use diffusion flame combustors with high amount of diluents to abate NOx to 15-25 ppmvd level. This program, which will reduce NOx from combustion of high hydrogen content IGCC fuels, is based on the Dry Low NOx (DLN) lean premixed approach for the combustion of natural gas with DLN. The lean premixed technique will be adapted to the challenging and unique demands of high hydrogen content fuels in an effort to achieve low NOx with elimination/reduction of the diluents that are currently required for NOx abatement of IGCC fuels. This will be accomplished by the design of an IGCC premixed combustor nozzle that is revolutionary in both its ability to accommodate fuels with high hydrogen content and at the same time deliver dramatically reduced emissions with no or minimum diluent injection.

B. Background/Relevancy

Background:

Emissions regulations for power plants have gradually become more stringent over the past few decades. This has driven interest towards gasification and gas turbines due to the potential for lower emissions and higher efficiency. Coal combustion in gas turbines is achieved by gasifying coal resulting in a mix of hydrogen, CO, nitrogen and other minor constituents. Depending on the gasification process, the relative proportion of hydrogen and CO can vary. Gas turbines utilizing these fuels are referred to as IGCC (Integrated Gasification Combined Cycle) machines.

IGCC fuels are currently burned in diffusion mode in gas turbine combustors. With diffusion combustion and diluent injection, current NOx guarantees for gas turbines utilizing IGCC fuels are still only as low as 25 ppmvd, with a few select offerings at 9 ppmvd. Reducing NOx by an order of magnitude requires a change in combustor design philosophy. In the past, natural gas combustion was first carried out in diffusion mode before premixed combustors were developed. This resulted in NOx guarantees dropping from about 25 ppmvd to 9 ppmvd. A similar evolution is needed for IGCC fuels to reduce NOx from 25 ppmvd towards the challenging DOE Turbine Program goal of 2 ppmvd.

Relevancy:

Achieving the goal of this program will constitute a significant engineering breakthrough and will set the stage for overall process improvements, broader application of gas turbines, and improve the economics of pre-combustion carbon capture concepts. IGCC combustion has been confined to diffusion combustors primarily because of the risks

involved in premixing hydrogen. Using only diffusion mode combustion, the only strategy that can be successfully used for NOx control to levels below 25 ppmvd remains diluent injection, which has limits both from a materials and chemical kinetics viewpoint.

Currently, most of the advances that are being made in gas turbine design are focused on premixed combustion. The achievement of a IGCC premixer design for hydrogen based fuels will enable the use of alternative premixed combustion approaches such as Late Lean Injection or Catalytic combustion for IGCC applications. Designing a premixer for IGCC fuels will advance the gas turbine combustion of pure hydrogen in premixed mode, and be a significant first step in overcoming the obstacles of operating with hydrogen as a fuel without compromising on efficiency or capital cost.

The significant benefit to the US public will be the development of environmentally friendly power plants and broader use of our abundant coal resource, both from the point of view of decreased source emissions and, potentially, fuel efficiency. The increased fuel efficiency can be translated to lower CO₂ emissions, which is a greenhouse gas. Further, increased availability will translate to lower costs of electricity to the US public.

Period of Performance: January 01, 2004 to June 30, 2005.

Executive Summary

This 18-month project translates DLN technology to the unique properties of high hydrogen content IGCC fuels, and will yield a design in preparation for a future testing and validation phase. Fundamental flame characterization, mixing, and flame property measurement experiments will be conducted to tailor computational design tools and criteria to create a framework for predicting nozzle operability (e.g., flame stabilization, emissions, resistance to flashback/auto-ignition). This framework is then used to establish, rank, and evaluate potential solutions to the operability challenges of IGCC combustion. The leading contenders are then studied and developed with the most promising concepts evaluated via computational fluid dynamics (CFD) modeling and using the design rules generated by the fundamental experiments as well as using GE's combustion design tools and practices. Finally, this project will scope the necessary steps required to carry the design through mechanical and durability review, testing, and validation, towards full demonstration of this revolutionary technology.

This project is being carried out in three linked tasks.

- 1. Develop conceptual designs of premixer and down-select the promising options.
- 2. Carry out CFD on chosen options (1 or 2) to evaluate operability risks.
- 3. Optimize design and reevaluate operability risks.

A series of fundamental experiments are planned and are being executed as part of realigned CA41448 "RAM" program Task 3 Combustion program being re-allocated to this High Hydrogen premixer program. These experiments will support Task 2 and 3 and will provide fundamental knowledge of premixed Hydrogen flame, resulting in better understanding of specific fundamental combustion phenomena deemed crucial to the development of robust premixers for IGCC applications

Task 1.0 – Develop conceptual designs of pre-mixer and down-select the promising options:

This task defined the "gap" between existing design capabilities and the targeted range of IGCC fuel compositions and evaluated the current capability of DLN pre-mixer designs when operated at similar conditions. Two concepts 1) swirl based and 2) multiple point lean direct injection based premixers were selected via a QFD from 13 potential design concepts. This task was completed and reported on in the previous semi-annual report.

Task 2.0 – Conduct CFD on chosen options (1 or 2) to evaluate operability risks:

This task developed the leading options down-selected in Task 1. Both lean direct injection concepts and a GE15 swozzle based premixer were examined by performing a detailed CFD study wherein the aerodynamics of the design, together with the chemical kinetics of the combustion process, was analyzed to evaluate the performance of the different concepts. The swozzle results identified potential problems with flame holding, flashback and adequate mixing. An effort to identify better swirler based premixers was initiated. To address flame holding issues for fuel injection from vanes or other flat surfaces, combustion laboratory testing was done to determine under what conditions a jet in cross flow would flame hold.

The laboratory test results showed that hydrogen has a very low tolerance to flame holding compared to methane, and that combustor pressure drop would have to be increased by about 1 percent to allow use a jet in cross flow injection method. CFD was also performed on fuel injection from a peg to simulate fuel injection off a vane's trailing edge. Further testing of this configuration was planned at GRC in Task 3 to determine if it could reduce flame holding concerns.

This task also contains combustion laboratory testing subtasks re-allocated and integrated from another DOE program to improve the underlying ability to model and evaluate NOx and hydrogen combustion as the accuracy of CFD NOx models has been limited:

Prostar default NOx models gave order of magnitude too high exit NOx values. H2 combustion models for Prostar had also not been well developed. Detailed 1-D analysis was performed to provide 1-step NOx and 1-step combustion models that could be utilized in CFD to provide more accurate estimates of NOx for more complicated combustion designs.

This task was concluded with a Conceptual Design Review of selected designs.

Task 3.0 – Optimize design and reevaluate operability risks:

This task extended the analysis of LDI concepts and increased understanding of the optimal design configuration. Designs were selected for testing at GRC. A CFD analysis of the planned GRC test rig was performed to ensure air entrainment would not interfere with test measurements.

In consideration of the disappointing CFD results for the GE15 swozzle, an evaluation of other premixed swirler designs was performed and the most promising one was selected for evaluation. Model development and CFD gridding of this model began. To validate CFD, a model of a similar swirler was run and compared with existing experimental results. So far, CFD accuracy in modeling species profiles and hence mixing has proven poor. Further model development is being done to improve accuracy.

In attempting to validate CFD NOx and H2 combustion models, comparisons were made between Fluent and Prostar software for both the LDI concept and premixed combustion using different combustion and NOx models. Results showed a significant difference in NOx depending on choice of software, combustion model, and NOx model. Efforts to further validate CFD NOx and H2 combustion models showed a significant difference in NOx depending on choice of software, combustion model, and NOx model. As experimental results from the laboratory LDI tests become available, the models will be further developed to improve accuracy.

This task also contains combustion laboratory testing subtasks re-allocated and integrated from another DOE program that will help further evaluate and optimize the selected conceptual premixer designs.

Experimental

This section presents a descriptive summary of the experimental methods in use for the conduct of this project. Described below are the experimental methods being used for the research efforts by Task, and where appropriate Sub-task, during this reporting period. Not all tasks/sub-tasks have yet been initiated during this reporting period of the program, and are so noted.

Task 1 - Develop conceptual designs of pre-mixer and down-select the promising options:

No experiments were designed or conducted to support this task.

<u>Task 2.0 – Conduct CFD on chosen options (1 or 2) to evaluate operability risks:</u>

Combustion Characteristics: Flame Holding

CFD modeling of swirler based configurations identified regions for possible flame holding. H2 jet in air crossflow tests were performed at GRC to identify flame-holding conditions. Figure 1 shows details of the test section for the experiment. There are two distinct parts to the test section: a fuel-air mixing tube, and a combustion chamber. The mixing tube is preceded by a contraction with a turbulence-generating screen. The mixing tube has a threaded fitting to allow easy replacement of fuel injectors to facilitate the screening of different designs. The fuel injector (FI) is located at the furthest upstream location in the mixing tube. Flashback sensors are positioned at three locations downstream from the fuel injector to identify the presence of flame in the mixing tube. The sensor assemblies consist of photomultipliers that are fibercoupled to the tube. Collimators are used to focus light emission from within the tube onto the end of the fibers. The sensors offer nanosecond time response and are used to trigger a fuel cutoff relay in the event of flame holding or flashback in the mixing tube. In normal operation, the fuel is injected and mixed with air in the mixing tube and a flame is ignited and stabilized in the combustion chamber. The combustor consists of an axially symmetric ceramic lined chamber. The flame is usually stabilized in the wake of a sudden expansion. The combustor is also instrumented with an emissions probe and a fast-response pressure probe to monitor combustion oscillations.

The fuel used in the experiment is a mixture of H2 and N2 in the ratio 60:40. For comparison with our baseline fuel, methane jets were also tested. For flame holding experiments, fuel was injected at an angle (θ) to the horizontal, axial flow of air. Two ignition sources were used to facilitate these tests - an upstream igniter placed in the contraction section, and an igniter placed near the combustor wall downstream of the mixing tube. In both cases, the optical sensors mounted on the side of the mixing tube were used to indicate the presence of flame. The sensors were coupled to a fuel cut-off relay that stopped the flow of fuel to the mixing tube to prevent overheating. A typical flame-holding experiment was conducted by starting the flow of heated air inside the mixing tube. The temperatures in the tube are continuously monitored through out the experimental procedure. The upstream igniter, which is a hydrogen torch, is then activated. Fuel is then turned on and kept flowing for a certain duration, after which the upstream igniter is then turned off. The flame temperatures are monitored to see the stabilization of the flame inside the mixing tube. The fuel is then turned off. The experiment is then repeated for higher fuel injection velocities.

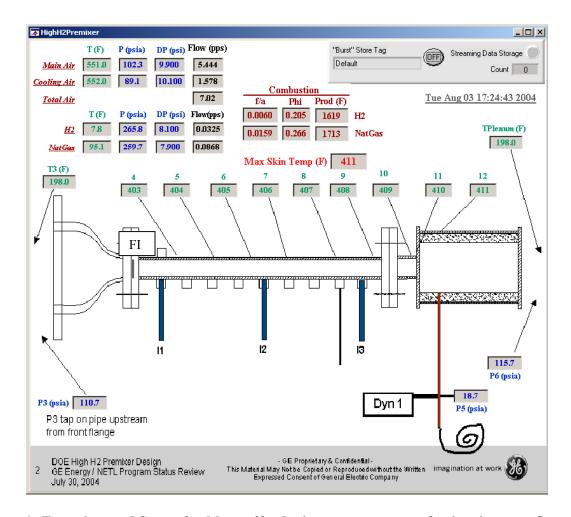


Figure 1: Experimental Setup for blow-off velocity measurements for jets in cross flow.

Task 3.0 – Optimize design and reevaluate operability risks:

Rig hardware was designed for tests of the LDI concept. These tests will use the same stand and equipment as was used for the flame holding tests. Similar to the flame holding rig, air will come in through an inlet section, Figure 2. The air will continue into a plenum section to the combustor while hydrogen goes through fuel lines passing through the air plenum, Figure 3, and connecting to an injection plate. The injection plate will have angled holes to inject the fuel into the air at the desired angle. The mixture will be ignited, temperature, emissions, and species profiles will then be obtained. Multiple injection plates will be made to allow for testing of different configurations.

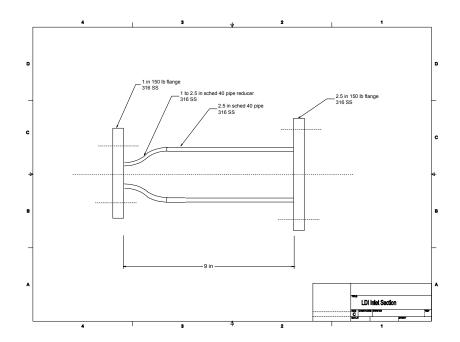


Figure 2: LDI Air Inlet Section

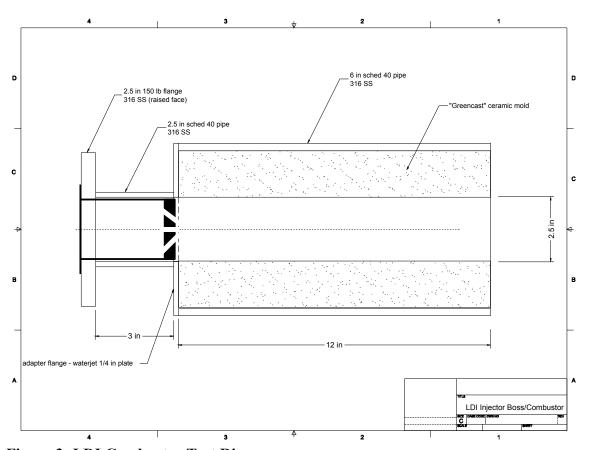


Figure 3: LDI Combustor Test Rig

Results and Discussion

The program status results are presented on a separate Task basis, as each of the five Tasks address separate areas of effort. Detailed task results are discussed for each active subtask, as appropriate, for activities during this reporting period. An overview section has been included to clarify each task's (and sub-task's) intentions, and to aid the understanding of progress to date.

Task 1 Status/Discussion:

Overview: A conceptual design review was conducted on February 27th 2004 to down-select premixer concepts for fuel with high Hydrogen content. Based on internal brainstorming and a review of prior literature and patents, a total of 13 premixer concepts were considered and rigorously evaluated for their expected performance and operational risks. A down-select process based on the 6-Sigma tools of Quality Function Deployment (QFD) and Pugh Matrix was used to arrive at two down-selected concepts of: (1) Swirl based premixers and (2) Multi-Point Direct Injection premixer concepts. In addition to the down-selection of 2 premixer concepts, a Failure Mode Evaluation Analysis (FMEA) was conducted to identify risks associated with these concepts, perform a risk evaluation, and finally propose risk mitigation strategies to contain these technical risks. Task 1 is complete and has been reported on in the previous semi-annual report.

Task 2 Status/Discussion:

Reaction Mechanism Validation

Previous analysis showed that the Hai Wang mechanism provided a good match with experimental data. Further analysis shows that a 1-step Marinov mechanism (H2 + O2 > 2H2O) provides a good match to Hai Wang (Figure 4). This 1-step mechanism is being evaluated for use in CFD to provide a computationally efficient means of modeling H2 combustion.

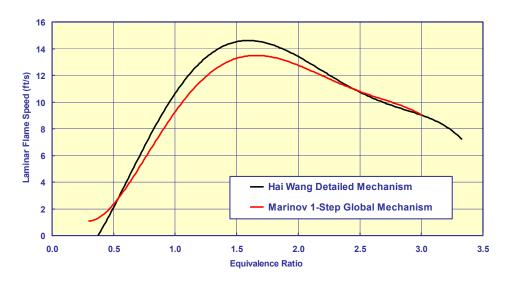


Figure 4: Laminar Flame Speed Comparison of Different Combustion Models

Validation of CFD NOx models with Chemkin Analysis

A simple CFD model of a H2/air burner (Figure 5) was developed using the Marinov 1-step reaction: H2 + 0.5O2 > H2O. The creation equation becomes:

 $k = 1.8E16exp(-17614/T) [H2][O2]^{1/2} kmol/sm3$

The exit temperatures values were then compared with equilibrium results to ensure a correct energy balance (Figures 6 and 7).

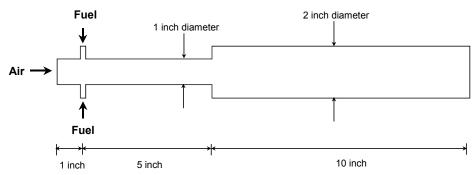


Figure 5: CFD Combustor Model for 1-Step Combustion Model Validation

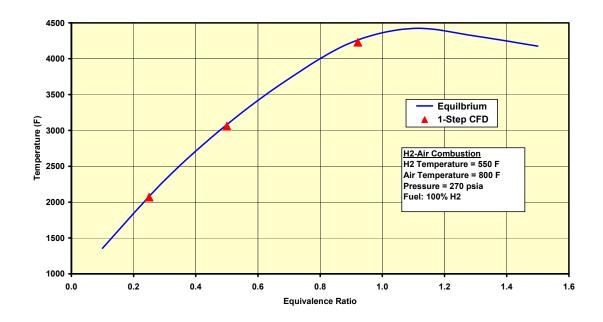


Figure 6: CFD Model Results Compared To Analysis For Pure H2

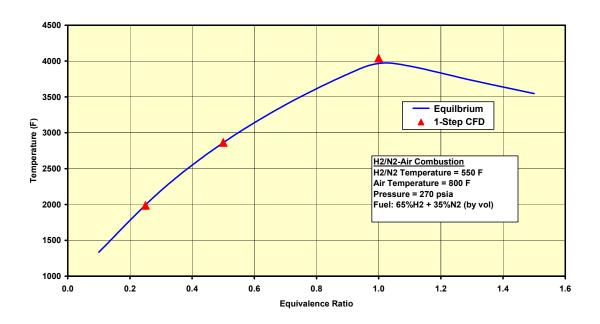


Figure 7: CFD Model Results Compared To Analysis For H2 Mix

A more detailed effort to match both Prostar and Fluent CFD results to experiment was begun using Sandia diffusion flame data and comparing temperatures, species profiles, and NOx concentrations. This effort will continue as part of Task 3.

Emissions Predictions

In order to predict expected NOx emissions for premixed H2 at gas turbine conditions, a model using a Perfectly Stirred Reactor (PSR) and a Plug Flow Reactor (PFR) was constructed as shown in Figure 8.

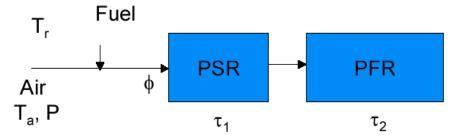


Figure 8: PSR/PFR Reactor Model

Initially, the rich and lean stability limits using a PSR were explored for the fuels of interest. The results are shown in Fig. 9a at gas-turbine conditions as a function of a characteristic flow residence time. The results confirm the increase in stability margin obtained by adding hydrogen to existing fuels for a range of residence times. Hydrogen combustion can be sustained even at

equivalence ratios close to 0.25, while limited hydrogen injection gives remarkable benefits in increasing blowout margin.

Emissions predictions from the PSR-PFR model corrected for 15% O₂ are shown in Figure 9b. Application of this approach for a particular combustor can be done by choosing the primary residence time to agree with lean-blowout data. Alternatively, if emissions measurements at one temperature are available then the PSR residence time may be chosen to agree with data, with predictions giving the parametric variations. If detailed flow-field predictions for the particular combustor are available, the primary-zone residence time can be approximately chosen to be an average turbulent residence time (Ck/e) in the stabilization zone. Limited experimental data on NOx emissions for pure H2 fuels in combustors are available and comparisons indicate differences in predictions with different chemical mechanisms and future work is warranted. However, a primary zone residence time of 0.1 ms was chosen for the calculation in Figure 10 to obtain agreement with lean-blowout temperatures for conventional combustors using methane as fuel. The secondary zone residence time was chosen to be about 3 ms. In Figure 9b, NOx and CO curves are shown for both rich and lean conditions as a function of flame temperature. The following conclusions are obvious from Fig. 9b:

- a) For the same flame temperature, combustion of pure hydrogen leads to higher NOx emissions than pure methane.
- b) Pure hydrogen fuels blowout at much lower temperatures than pure methane.
- c) Although hydrogen blows out at lower equivalence ratios, blends of hydrogen and nitrogen blow out at temperatures even lower than pure hydrogen due to dilution effect on temperature.
- d) Addition of hydrogen to methane leads to a significant drop in lean blowout temperatures.

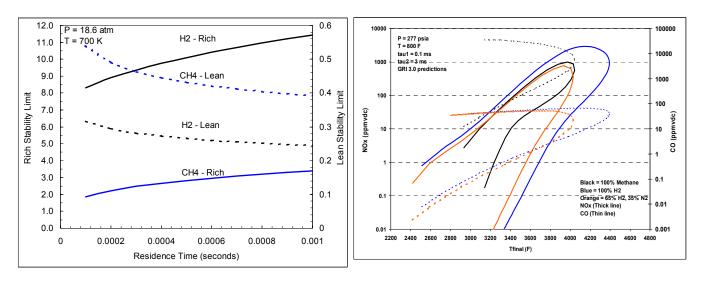


Figure 9 a, b: Stability and emissions predictions using GRI 3.0, Dryer, Wang mechanisms for hydrogen, methane, and methane/hydrogen mixtures.

Figure 10 shows NOx model results compared to experimental data as a function of temperature for pure hydrogen. The experimental data though is at temperatures below the region of interest. The match at these temperatures isn't very good and the model results indicate that even for a premixed H2 fuel, NOx may be above goal. Premixed H2 combustion tests will be performed at GRC to explore this further.

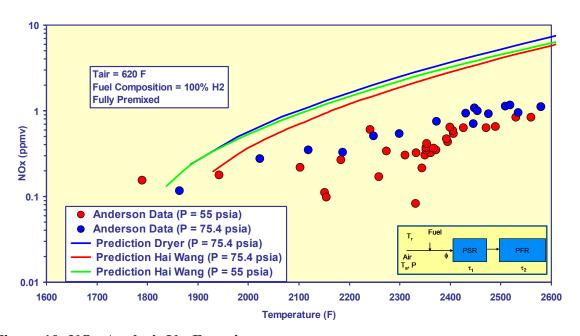


Figure 10: NOx Analysis Vs. Experiment

Prostar's built in NOx model has previously been seen to provide NOx estimates orders of magnitude too great. To provide a NOx model for CFD calculations, the PSR/PFR method is used based on the PSR and PFR time scales estimated from a typical CFD model, Figure 11.

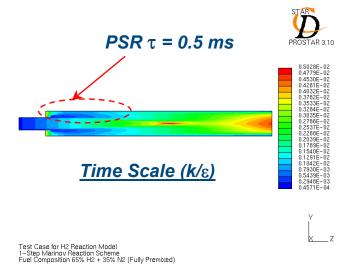


Figure 11: CFD Premixed H2 Combustion Model

The results are then used to determine the constants for a 1-step thermal NOx model - N2 + O2 > 2NO. The NOx generation equation for the CFD models becomes:

$$k = (4.55573E11e(-49455.1/T) [N2][O2]^{1/2})/T^{1/2} \text{ kmol/sm3}$$

Figure 12 compares the results from a Prostar CFD model using both the 1 step combustion and 1 step NOx model for a premixed fuel/air mixture entering the reactor shown in Figure 11 with the PSR/PFR model results over temperatures of interest.

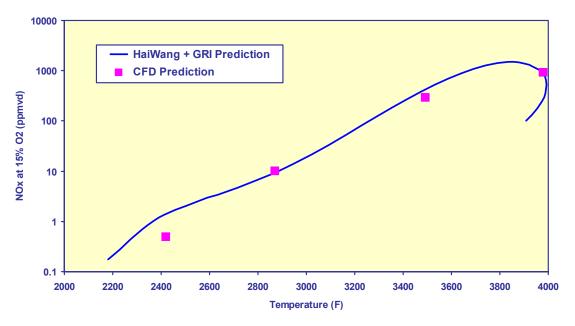


Figure 12: CFD Results Vs. Analysis

GE 15 Swozzle CFD

To model a swirl based premixer, a pre-existing GE 15 model was used. The swozzle had a 45° vane angle, a 1.25" hub diameter, 2.088" shroud diameter and 8 vanes per swozzle. The model assumed a uniform inlet velocity profile, steady state compressible flow, k-e turbulence with 2-layer model on the vane. A fuel mix of 65% H2 and 35% N2 was injected through faces in the vanes and the inner hub. Figure 13 shows the mesh and model.

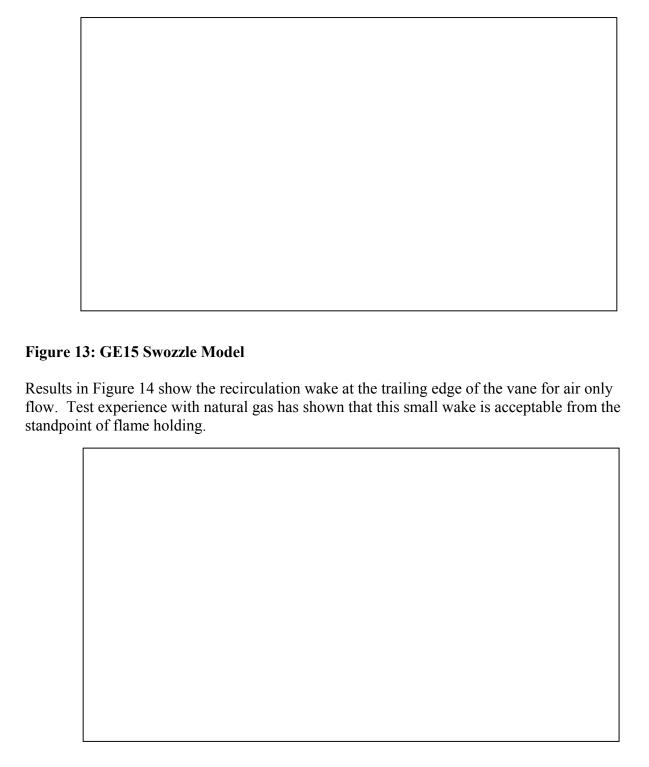


Figure 14: GE 15 Air Only Flow Model

Figure 15 shows the recirculation wakes trailing the fuel injectors. Each wake is a potential flame holding region. It is expected that results from the GRC flame-holding tests will determine whather these walkes are chiestianable.

whether these wakes are objectionable.

Figure 15: GE15 Swozzle Fuel Injected into Air Flow Model

Figures 16 and 17 show the fuel/air ratio moving through the swozzle and then continuing downstream. As can be seen, significant non-uniformity exists even well downstream of the vane. It is expected that mixing could be improved by optimization of this design, but as explained below, the potential flame holding and flashback issues for this design have led to a refocus on a different swirler concept. Thus no further optimization of the swozzle was undertaken.

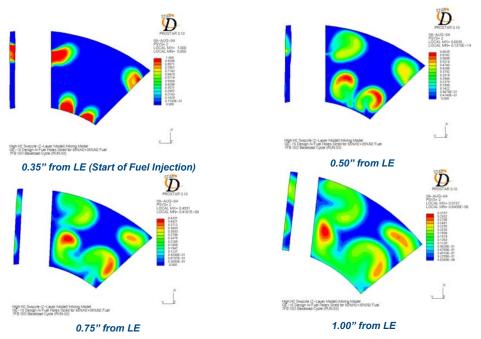


Figure 16: F/A Ratio GE15 Swozzle

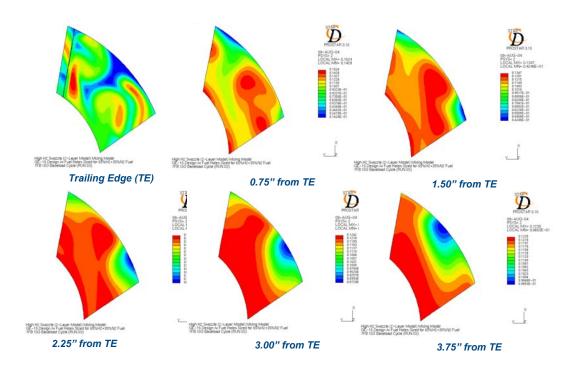


Figure 17: F/A Ratio GE15 Swozzle (cont.)

The flow in the downstream burner tube was also examined to determine the possibility of flashback. Boundary layer flashback is assumed to occur for a flammable mixture if (du/dy)qD/sL < 1. An assumption was made that the quenching distance was the same as for 100% H2 at standard conditions and that the flame speed was the maximum predicted laminar flame speed. This is expected to be a conservative evaluation of flashback potential, since quenching distance for a H2/N2 mixture at elevated pressure and temperature will be less than for pure H2 at standard conditions. Previous validation of this methodology provided some confidence in the predictions. Figure 18 shows equivalence ratio and (du/dy)qD/sL in the burner tube downstream of the swirler. As can be seen, flashback is very likely.

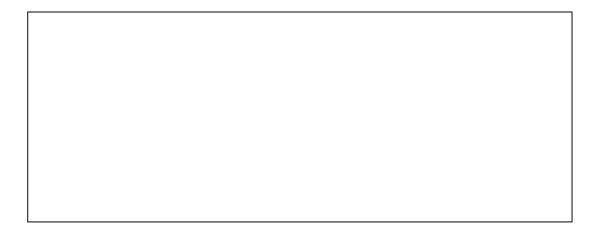


Figure 18: Flashback Criteria in Burner Tube

Due to all of these limitations (flame holding, flashback, poor mixing), Task 3 focus has moved into looking at other swirler configurations as well as eliminating the burner tube to reduce flame holding surface. Further modeling and experimental studies were also done to determine if changing injection angle could reduce flame holding.

Jet in Crossflow CFD

Figure 19 shows a CFD model of a jet in crossflow at two different injection angles. A lower angle shows less recirculation behind the jet, possibly resulting in reduced flame holding. This though appears to contradict what was actually seen in the GRC flame holding studies.

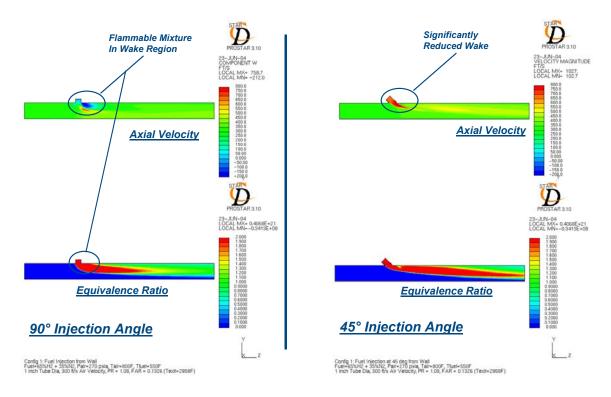


Figure 19: Fuel Injection At Varying Angles

Peg Injection CFD

As a possible means of minimizing flame holding and examining possible swirler and peg injector configurations with fuel injection off the trailing edge, CFD was performed on a wedge with varying wedge angles to minimize recirculation zones and with varying fuel injection angles to minimize flame holding. Figure 20 shows the impact of wedge angle on recirculation zones.

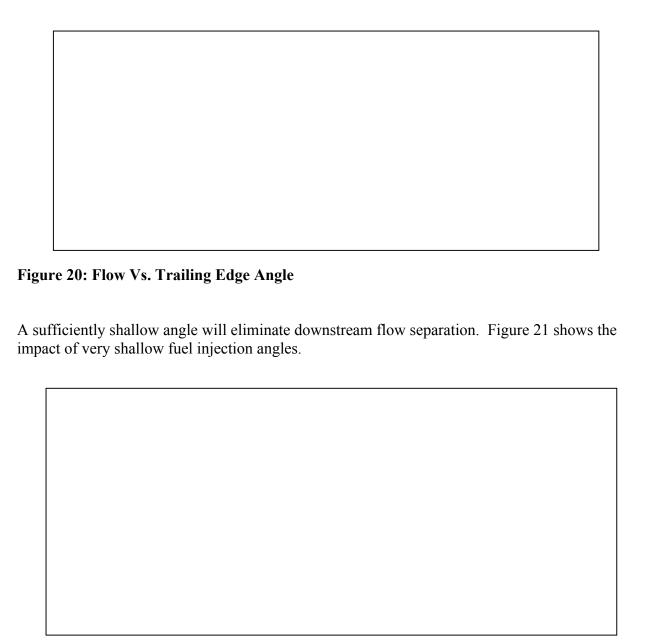


Figure 21: Fuel Injection off a Trailing Edge

A low enough angle may reduce flame holding. However, fuel mixing could be reduced, resulting in higher NOx, Figure 22. A 28° fuel injection angle with a 5.5° wedge angle appears to be a potentially reasonable configuration. Testing at GRC as part of Task 3 will examine the flame for a peg type injector further.



Figure 22: Fuel Mixing off Trailing Edge Fuel Injection

LDI CFD

To eliminate concerns with flame holding, the concept of direct injection was examined. If injectors of a small enough size could be used to allow for mixing on a very short time scale, the NOx formation could be low. Three basic configurations were explored, Figure 23. The first is one fuel jet and one air jet each angled toward the other; the second is two fuel jets injecting into one air jet, the third is four fuel jets injecting into one air jet.

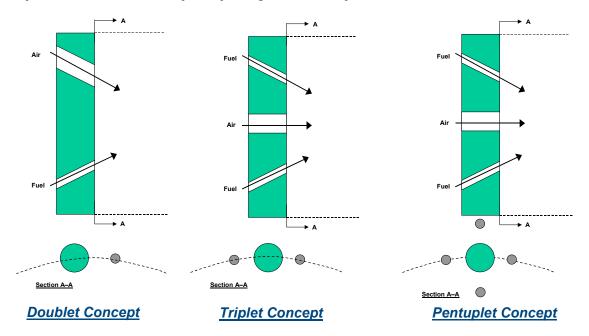


Figure 23: LDI Concepts

Figure 24 shows equivalence ratio and temperature through a slice of the combustor for each concept. As can be seen, the doublet skews to one side because the air jet is larger than the fuel jet and pushes it to the side. The triplet has a larger volume high temperature region than the other concepts. This impacts relative NOx as seen in Figure 25 and 26. The NOx values here are obtained using Prostar's default NOx model and are believed to be at least an order of magnitude too high but are used at this point to make a relative comparison of the concepts. Based on this, for a constant air injector diameter, the pentuplet appears to provide the best performance for a standalone injector. A more detailed modeling effort is made as part of Task 3.

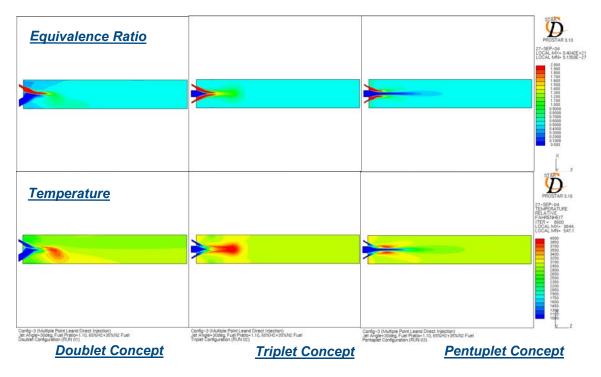


Figure 24: LDI Equivalence Ratio and Temperature

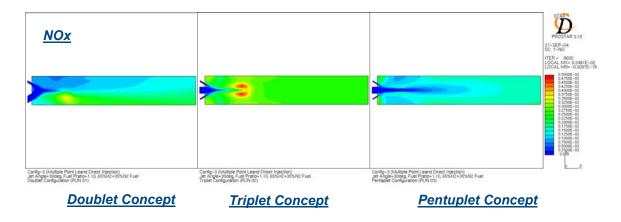


Figure 25: LDI NOx

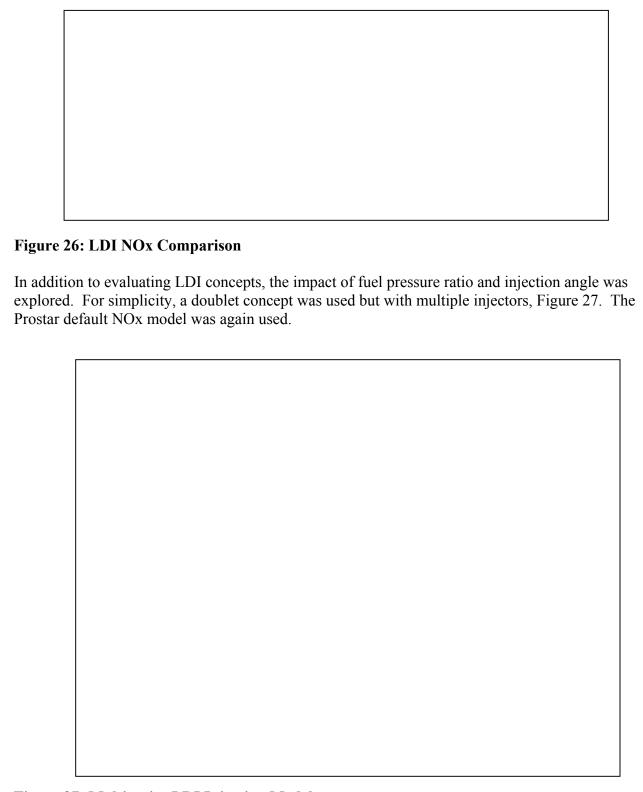


Figure 27: Multi-point LDI Injection Model

Figures 28 and 29 show the relative NOx performance. The results indicate that a lower injector angle (off the injector plate) and a higher pressure ratio gives a lower NOx value. This appears to be due to better mixing from a sharper injection angle and higher fuel velocity.

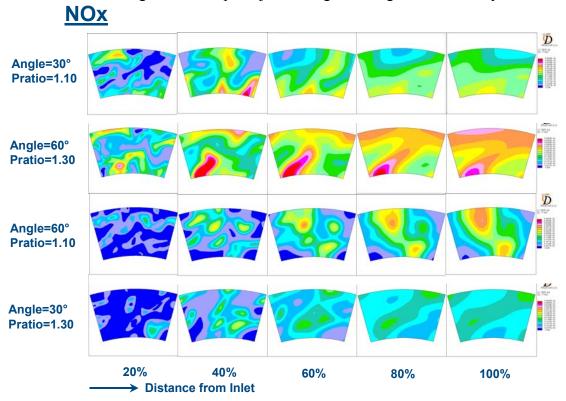


Figure 28: LDI Profiles Downstream

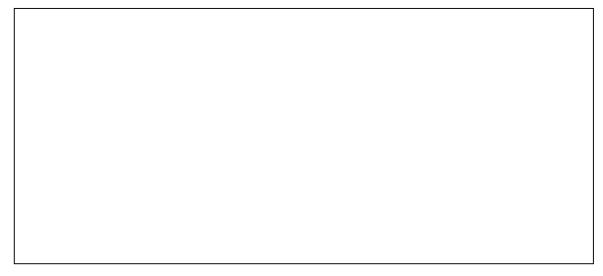


Figure 29: LDI NOx for Varying Injection Angle and Fuel Pressure Ratios

GRC 2.1 Combustion Kinetics Modeling

See previous sections: Reaction Mechanism Validation, Validation of CFD NOx models with Chemkin Analysis, and Emissions Predictions with CFD.

GRC 2.4 Combustion Characteristics

Flame holding tests

As discussed earlier, CFD models of the GE15 swozzle design showed potential for flame holding. To avoid this process, design requirements stipulate that the average velocity in the premixing tube be much higher than the turbulent burning velocity of the mixture.

Hydrogen has a burning velocity that is about 6-7 times that of methane under gas-turbine conditions of interest. This can lead to significant air-velocity requirements in the premixing tube. The maximum air velocities in the combustor are limited by pressure drop. Typical swirl-stabilized combustors operate at pressure drops about 3-5% of the operating pressure across the combustor.

The stability of jets in cross-flow has been studied for hydrocarbon flames [1-3]. Based on these studies, two stability limits were identified as shown in Figure 30, with flame holding defined by the enclosed area between the two curves. Although this curve has not been verified to hold for hydrogen flames, there is recent evidence that mixtures of methane and hydrogen could conform to a similar theory should proper burning velocities and equivalence ratios be used. These tests examine the blowout behavior of hydrogen and methane jets in cross flow under pressures and temperatures of interest. The critical-blowout velocities of the fuel jet in this configuration will provide data for the minimum-air velocities to avoid flame holding and motivate theories for better design of flame holding experiments for practical fuel-injection configurations.

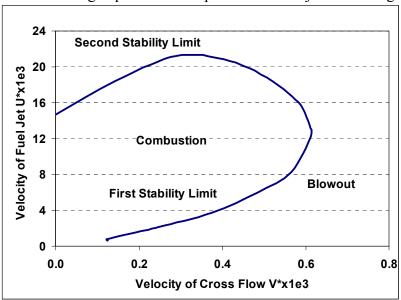


Figure 30: Universal non-dimensional stability curve for jets in cross-flow for methane & propane [2]

As described earlier in the Experimental Setup, air then fuel flows into a mixing tube and is ignited. The igniter is turned off and the flame temperatures are monitored to see the stabilization of the flame inside the mixing tube. The fuel is then turned off. The experiment is then repeated for higher fuel injection velocities. Table 1 shows the list of runs.

Table 1: Summary of Experimental runs on flame holding

Data	Test File	Injector	Injection	Air	Fuel	Fuel
Set		diameter	Angle	Properties	Composition	Temperature
		(in)	(deg)		(Vol)	(F)
A	10/12/2004	0.159"	60°	57.5 psia	60% H2,	60 - 70 F
				675 F	40% N2	
В	10/19/2004	0.159"	90°	57.5 psia,	60% H2,	60 - 70 F
				740 F	40% N2	
C	10/20/2004	0.159"	45°	57.5 psia,	60% H2,	60 - 70 F
				740 F	40% N2	
D	11/2/2004	0.080"	90°	57.5 psia,	60% H2,	60 - 70 F
				740 F	40% N2	
Е	11/3/2004	0.080"	45°	57.5 psia,	60% H2,	60 - 70 F
				740 F	40% N2	
Е	11/4/2004	0.159"	45°	57.5 psia,	60% H2,	60 - 70 F
				740 F	40% N2	
F	11/16/2004	0.5"	90°	58 psia,	100% CH4	60 - 70 F
				720 F		
G	11/17/2004	0.159"	90°	240	60% H2,	60 – 70 F
				psia,	40% N2	
				783 F		
Н	1/5/2005	0.159"	-45°	63.7	60% H2,	60 – 70 F
				psia,	40% N2	
				687 F		

Based on the temperature records during this process, two well-defined events are recorded for each run as shown in Figure 31. A flame holding event is defined to occur if the flame-tube thermocouples record significantly higher than inlet readings (about 200 ° F), even after the igniter is turned off and the high temperature readings in the flame tube persist until the fuel is turned off. This suggests self-sustained flame stabilization in the mixing tube. A blowout event is defined to occur if the flame-tube thermocouples record a sharp drop in temperature immediately after the igniter is turned off, suggesting that a flame can be sustained in the mixing tube only with continued presence of an ignition source.

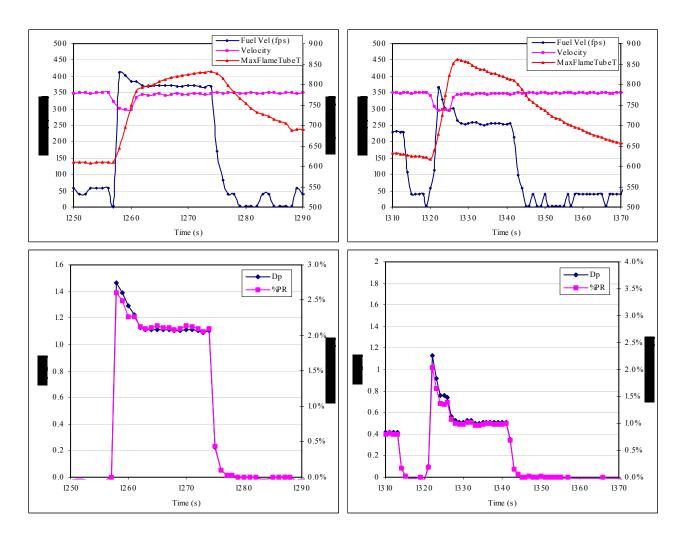


Figure 31: Transients of maximum temperature in the flame tube, fuel-jet velocity, air-flow velocity, pressure drop and pressure ratio across the fuel injector for hydrogen injection at 90° angle to the main air flow. Panels (a) and (c) correspond to flame holding regime and panels (b) and (d) correspond to blowout regime.

The blowout experiments were performed for 60/40 H2/N2 mixtures and pure CH4 in air for initial pressures between 3 atm and 14 atm, temperatures between 260°F and 800°F and a jet diameter of 0.159" (4.04 mm). The experiments were performed with a constant air flow and by decreasing the fuel-flow velocities until the blowout event occurred. The experiment was then repeated at different air flow velocities. The velocities of fuel jets and air flow have been normalized by the characteristic velocity

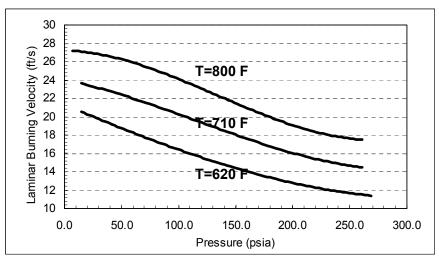
$$W = S_U \left(\frac{HS_U}{V} \right) \left(\frac{\rho_{\infty}}{\rho_{\alpha}} \right)^{1.5},$$

where S_U refers to the maximum laminar burning velocity at the conditions, H refers to height at which the mean fuel mass-fraction falls to stoichiometric value, v is kinematic viscosity of fuel gas, ρ_{∞} density in the free stream, ρ_e density of fuel flow.

The lift-off height is defined by the expression

$$H = \left[4 \frac{Y_e}{Y_s} \left(\frac{\rho_e}{\rho_\infty} \right)^{1/2} - 5.8 \right] d_e,$$

where Y_e and Y_s refer to fuel mass fractions at jet exit and at stoichiometric conditions and d_e is the fuel-jet diameter. A key parameter for calculation is the maximum laminar burning velocity of the mixture, which was calculated using detailed chemical kinetic mechanisms in a freely propagating flame configuration. For this case, the maximum laminar burning velocities for the 60/40~H2/N2 mixture were calculated at the conditions of interest and shown in Figures 32a and 32b below.



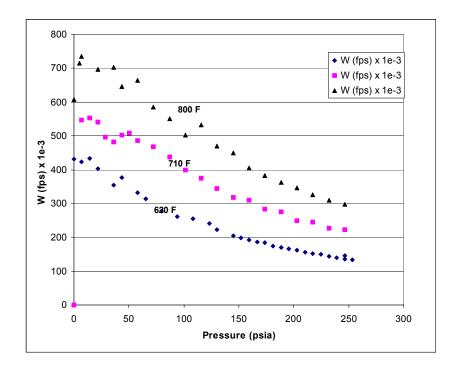


Figure 32 a, b: Maximum laminar burning velocities and calculated characteristic velocities (W) at the conditions of interest for 60%H2 40%N2 mixtures

Using these velocities, the experimental data were plotted in the universal flame holding parameters for both methane and hydrogen as shown in Figure 33 below. While the results for methane are close to the first stability limit of the universal flame holding curve, the results for hydrogen do not agree with the universal curve and lies far to the right. Thus hydrogen has a low tolerance for flame holding compared to most other hydrocarbons.

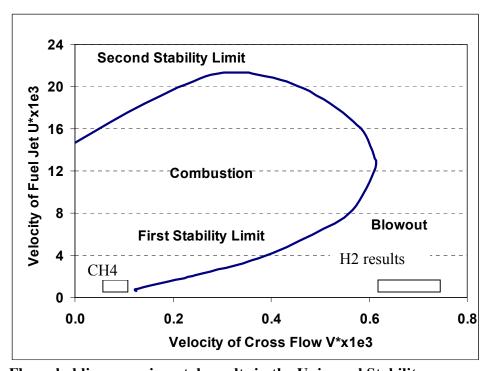
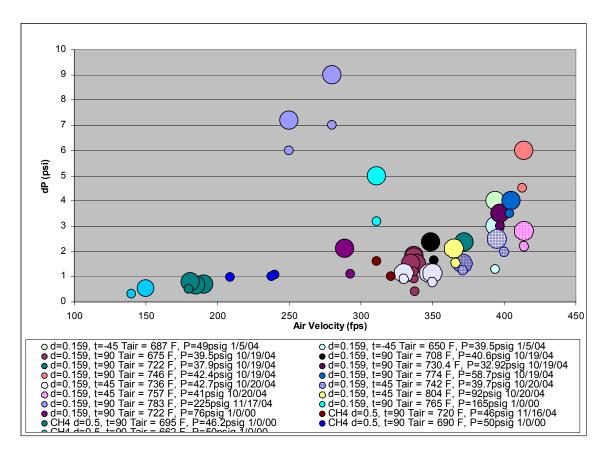
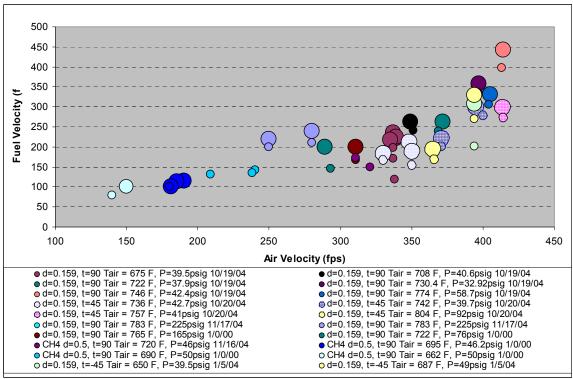


Figure 33: Flame holding experimental results in the Universal Stability curve coordinates.

The flame holding results in physical coordinates are shown in Figure 34 below. In the figure, only the marginal flame holding data are shown although experiments were conducted with progressively decreasing fuel-jet velocities until blowoff conditions were reached. The results for 45° injection are shown by the hatched circles. Two cases were performed for fuel-injection in the upstream direction at injection angles of -45°. Results from methane jets are also shown for a larger jet diameter, 0.5" (12.7 mm), since for smaller jet diameters flame holding was not observed. The data in the figure seems to follow the first stability limit with respect to Figure 30. The second stability limit was not observed with this experimental setup, since for high fuel jet velocities, downstream flame stabilization in the dump combustor was observed.





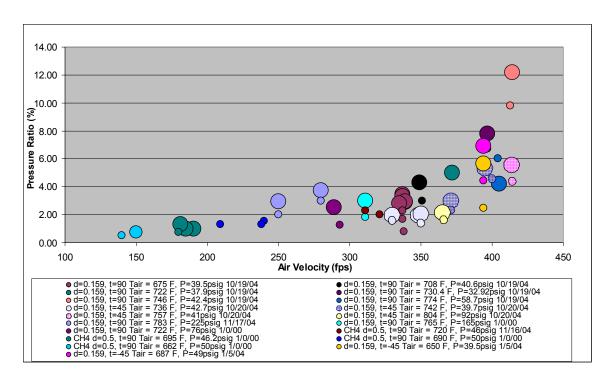


Figure 34a,b,c: Marginal curves for blow-off of jets in cross flow – Fuel jet velocities, dPs(psi), and pressure ratios.

From the results in Figure 34 above, the following conclusions can be made:

- 1. A mixture of 60%H2, 40%N2 has a low tolerance to flame holding compared to methane. The methane experiments were performed with 0.5" injector compared to 0.159" injector with hydrogen. For methane-air mixtures, flame holding was not observed for air velocities above 200 fps, although experiments were conducted up to air velocities of 325 fps. This suggests that hydrogen has a very low tolerance to flame holding with respect to methane.
- 2. The flame holding margin for 45° injection was lower than the flame holding margin for 90° injection and the results for –45° injection was comparable to the other cases (90° and 45°).
- 3. The effect of injection angle on flame holding margin is negligible.

These results indicate that, for mixtures of hydrogen of 60% or greater, a jet in crossflow is most likely not an acceptable method of introducing the fuel into the airstream, for air velocities consistent with current gas turbine combustor pressure drops. To be useable, the air velocity would need to be increased to at least 400 ft/sec, which implies an increase of about 1 percent in combustor pressure drop. For this reason, further testing will be conducted with the so-called peg injection scheme, as described in the Task 2 CFD analysis section above.

GRC 2.2 Laminar Flame Measurements and GRC 2.3 Mixing Studies

Based on the results of both literature searches and plans to move ahead with testing injector concepts at GRC as part of task 3 it was concluded that both tasks GRC 2.2 and 2.3 should not be done. Mixing studies are still planned for Task 3 at the current time.

Task 3 Status/Discussion:

Overview: Further efforts to develop and examine NOx models for CFD were made. An extensive look at the impact of different models and operating conditions on NOx for the LDI concept was performed. Examination of LDI concepts continued in Task 3. A decision was made on which LDI concepts should be explored further in testing at GRC. An evaluation of different existing swirler concepts was performed and a decision was made to further examine a GE Aircraft twisted DACRS nozzle. As part of this, the CFD of the standard DACRS configuration was performed using GE Aircraft's pre-existing CFD models in an attempt to improve the match between CFD and GE Aircraft's test data for this nozzle. A simplified CFD model of the GRC rig to be used for LDI testing was performed to ensure air entrainment would not be an issue for the planned test configuration. Further validatation of CFD NOx models was begun by attempting to match Sandia H2 combustion results against CFD models. All of these tasks will be continued in the next reporting period.

GRC LDI CFD

Due to personnel changes and a management decision to focus on Fluent CFD software, further evaluation of LDI concepts were looked at in Fluent. Figure 35 shows a comparison of the triplet and pentuplet concepts on a flow scale GRC could use for testing. In addition to the earlier evaluation, fuel in the center with air on the outside was modeled as well as the effect of varying scale. All of the models used a 1.3 fuel pressure ratio and a 30° injection angle (off the injector plate) for the outer jet. NOx was examined based on the Fluent default model. From Figure 33, we see that NOx is lower with the fuel jets on the outside and is lower for the smaller scale jets.

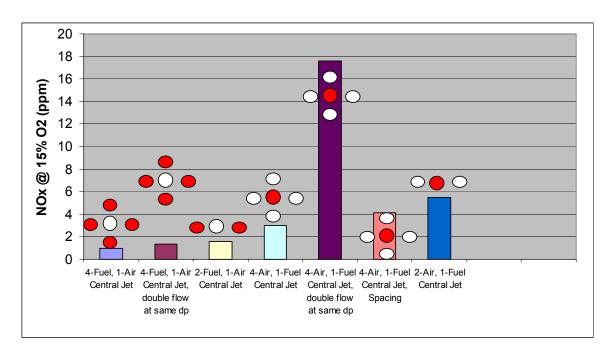


Figure 35: NOx Comparison for Different LDI Concepts

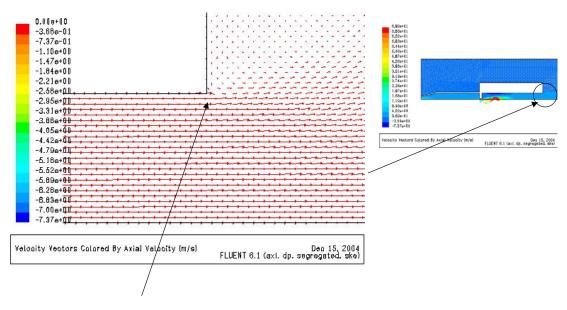
Based on these results, a downselect for testing the LDI concept was made, Table 2. The initial tests will consist of five configurations, all with air in the center and fuel outside. Both pentuplet and triplet configurations will be examined at two different scales. The baseline flame temperature will roughly match GE's 7FB but equivalence ratio will be higher to make up for the lower air and fuel temperatures GRC is limited to. The fuel injection angle will be 30° for each test but a lower fuel pressure ratio test will be run. Pressure, temperature, and equivalence ratio will all be varied for the given configuration to determine their impact. Testing at GRC of the NOx for a premixed combustor is also being considered.

Table 2: GRC LDI Test Configuration

Fuel Composition	65%H2/35%N2	65%H2/35%N2	65%H2/35%N2	65%H2/35%N2	65%H2/35%N2
Tflame (F)	2958	2958	2958	2958	2958
FAR	0.1461	0.1461	0.1461	0.1461	0.1461
No. Air Holes	1	1	1	1	1
(center)	ı	ı	ı	ı	!
No. Fuel Holes	4	2	4	2	4
(outer)	7	2	7	2	7
Pair (psia) (static)	90	90	90	90	90
Tair (F)	700	700	700	700	700
Pfuel (psia)	117.0	117.0	96.6	117.0	117.0
Tfuel (F)	100	100	100	100	100
Air Flow (lbm/s)	0.1004	0.0999	0.1997	0.1997	0.1997
Air dP/P, %	2.0%	2.0%	2.0%	2.0%	2.0%
Fuel Flow (lbm/s)	0.015	0.015	0.029	0.029	0.029
Fuel dP/P	1.30	1.30	1.07	1.30	1.30
Outer jet angle	30	30	30	30	30

GRC LDI Rig CFD

During GRC's flame holding test an emissions measurement was made. The results showed air entrainment into the back end of the combustor. This would impair our ability to accurately measure NOx for the LDI experiments. To ensure the LDI rig design wouldn't experience entrainment, a 2D axisymmetric CFD model of the rig was run over a range of temperatures and velocity. As seen in Figure 36, no entrainment was found.



No backflow into the combustor

Figure 36: LDI Rig CFD Model

GRC LDI CFD Part 2

In the initial GRC LDI CFD, the models were run using expected lab air and fuel temperatures but without compensating with a higher equivalence ratio. This resulted in lower flame temperatures than desired and hence lower NOx. To gain a better idea of the impact of higher flame temperatures, the triplet model was rerun using both the lower air and fuel temperatures but at a much higher equivalence ratio and using higher air and fuel temperatures and a slightly higher equivalence ratio to match 7FB conditions. As can be seen in Table 3, depending on NOx model assumption as well as how flame temperature is matched, outlet NOx could range from 30 to 261 ppm. However, while these new models have the right temperature, since they used the earlier configuration, they have different pressure ratios and hence different mixing ratios. The Table 2 test configurations have been sized to ensure both the correct flame temperatures and pressure ratios. CFD of these configurations will be carried out to more accurately model NOx.

Table 3: NOx LDI Comparison's For Different Combustion and NOx Models

	-			NOx (ppm): 1	NOx (ppm):	NOx (ppm):
				step NOx model	Fluent NOx	Fluent NOx
		1 step	PDF combustion	w. 1 step	model w. 1 step	model w. PDF
	phi	combustion Tout	Tout	combustion	combustion	combustion
GRC Scale Triplet						
(lower phi and GRC air						
and fuel temps)	0.524	1688	2579	12	2.4	2
GRC Scale Triplet						
(matching 7FB temp by						
matching 7FB gas						
temps and phi)	0.546	1929	3013	261	68	57
GRC Scale Triplet						
(matching 7FB temp T						
by increasing phi)	0.673	1916	2989	140	30	31
GRC Scale Triplet						
(matching 7FB temp T						
by increasing phi)						
using 2nd diff for						
everything	0.673	1916	2989	145	35	NA

Fluent/Prostar NOx model comparisons:

In an attempt to better compare Fluent results with Prostar results and to gain a better estimate of expected NOx values to be obtained during GRC testing, the Task 2 pentuplet model was rerun in Prostar, this time using the 1-step NOx model developed earlier and was also rerun in Fluent. This model though at a slightly smaller scale also has the advantage of being closer to the desired flame temperature and pressure ratios than the previous GRC LDI models. Table 4 shows the results. NOx here ranges from 42 to 154 ppm. Runs have also been done to look at the impact of inlet turbulence values, using second order vs. first order differencing, and double vs. single precision. The impact of all of these factors is small. The choice of NOx model though is not, and unlike the last example, the choice of combustion model.

Table 4: NOx Fluent/Prostar Comparison

	phi	Outlet T (F)	NOx (ppm)
Fluent 1 step			
combustion, 1 step			
NOx	0.546	3000	154
Fluent 1 step			
combustion, 1 step			
NOx - low (default)			
inlet turbulence	0.546	3000	144
Fluent 1 step			
combustion, Fluent			
model NOx	0.546	3000	97
Fluent 1 step			
combustion, Fluent			
model NOx - low			
(default) inlet			
turbulence	0.546	3000	86
Fluent PDF			
combustion, Fluent			
NOx model	0.546	3000	42
Star w 1 step NOx, 1			
step combustion	0.546	2993	63

The NOx for the premixed fuel combustor, previously described in Task 2, was also compared between the Fluent and Prostar and between Fluent's default NOx model and the NOx 1-step model. Table 5 shows this comparison for 1 operating point. Again, there is a significant degree of variation with model with the Fluent model giving consistently lower NOx values. Prostar using the same combustion and NOx models gives lower NOx than Fluent again as well.

Table 5: Premixed Fuel NOx Model

	phi	Outlet T (F)	NOx (ppm)
Fluent 1 step			
combustion, 1 step			
NOx	0.5	2871	19
Fluent 1 step			
combustion, Fluent			
model NOx	0.5	2871	3.2
Fluent PDF			
combustion, Fluent			
NOx model	0.5	2863	2.3
Star w 1 step NOx, 1			
step combustion	0.5	2869	9.4

Clearly, there is significant variation based on choice of CFD code, NOx model, and combustion model. Once experimental combustion studies are complete at GRC, as part of Task 3, a multistage PFR/PSR model will be developed to in turn provide a more accurate model for use in the CFD codes at the temperatures and conditions of interest. In addition, an effort is currently in process to match experimental NOx results from Sandia using various kinetics models. This is described in the following section.

Sandia Flame Match Modeling

Sandia National Laboratories has measured species and temperature profiles along a hydrogen diffusion flame. To continue to validate CFD models, this flame is being modeled in both Prostar and Fluent using different combustion and NOx models. Once complete, these models will be compared with the Sandia results and along with the multistage PSR/PFR used to improve the CFD NOx models.

Swirler Downselect

Since the earlier GE15 swozzle didn't appear promising in this application, other swirler concepts were considered. The Pugh matrix in Table 6 shows the results of this evaluation. The twisted DACRS concept, shown in Figure 37, was judged most promising. This is a counter rotating swirler with a twisted inner vane to minimize separation off the inner hub. This design utilizes injection from the trailing edge of the swirler vane, as in the peg injection analyzed in Task 2. It is expected that this will significantly reduce flame holding propensity; testing is planned at GRC to validate this expectation. A model of the swirler was obtained from GE Aircraft and work has begun to model it with CFD.

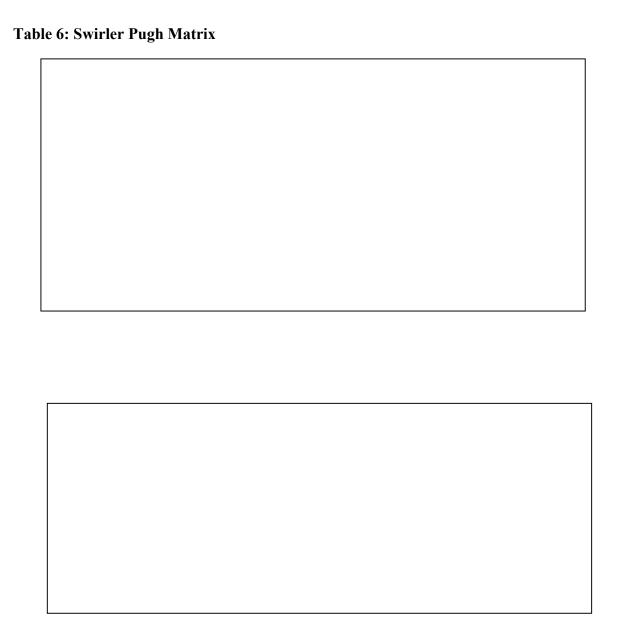


Figure 37: DACRS Nozzle

DACRS CFD Modeling

GE Aircraft had previously performed CFD modeling on the standard DACRS nozzle. They were unable to obtain a good match between the CFD methane species profile and experimental results. Figure 38 shows the mixer exit profile concentration radially for both CFD and experiment. Even though methane is injected from the outer vanes and outer hub, the experimental results indicate that much of the methane has moved to the center by the time it exits the mixer. CFD results do not agree.

Figure 38: DACRS Nozzle CH4 Concentration:

Since results are likely to be similar for the twisted DACRS nozzle, we obtained a copy of GE Aircraft's DACRS CFD model and varied grid density (Figure 39) and turbulence model (Figure 40) in an effort to obtain results closer to experiment. So far we haven't improved upon GE Aircraft's results. Attempts to do Prostar models, 360° models, and a full LES simulation are being considered.

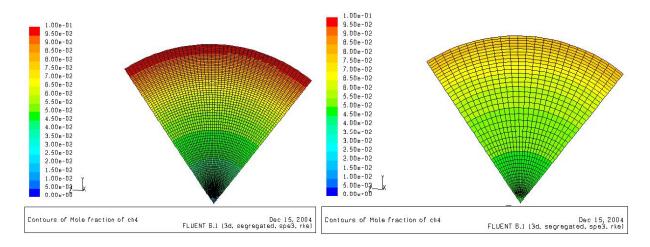


Figure 39: Grid Density Effect on DACRS Exit CH4 Concentration

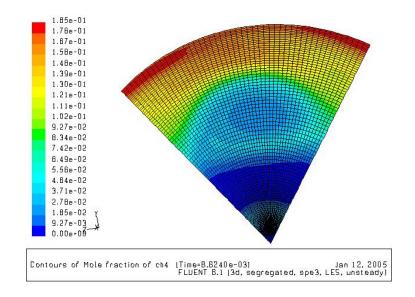


Figure 40: Impact of LES on DACRS Exit CH4 Concentration

Conclusions

Task 1 - Develop conceptual designs of pre-mixer and down-select the promising options:

The Task 1 Conceptual Design Review (CDR) of potential high Hydrogen premixer designs is complete. Two designs down-selected via a QFD from 13 potential design concepts are: (1) swirl based premixer and (2) multiple point lean direct injection based premixer.

Task 2.0 – Conduct CFD on chosen options (1 or 2) to evaluate operability risks:

This task developed the leading concepts down-selected in Task 1. Both lean direct injection concepts and a GE15 swozzle based premixer were examined by performing a detailed CFD study wherein the aerodynamics of the design, together with the chemical kinetics of the combustion process were analyzed to evaluate the performance of the different concepts. The GE15 swozzle results identified potential problems with flame holding and flashback. The swozzle also failed to provide adequate mixing. An effort to identify better swirler based premixers was initiated. To address flame holding issues for fuel injection, testing was done at GRC to determine under what conditions a jet in cross flow would flame hold. Results showed that hydrogen has a very low tolerance to flame holding compared to methane, and that combustor pressure drop would have to be increased by about 1 percent to allow use of this injection method. CFD was also performed on fuel injection from a peg to simulate fuel injection off a vane's trailing edge. Further testing of this configuration was planned at GRC to determine if such a configuration could reduce flame holding concerns.

CFD analysis of the LDI concept was begun in this task, but initial results did not allow selection of a final configuration. It was planned to perform further analysis in Task 3, prior to selecting a small number of concepts for testing at GRC, which would allow validation of the CFD tools for further optimization of this design.

Since CFD models were not giving good NOx estimates, 1-D chemical analysis was used to develop better NOx and combustion models that could then be utilized in CFD to provide more accurate estimates of NOx.

This task was concluded with a review that provided all the results save for the GRC flame holding experiments.

Task 3.0 – Optimize design and reevaluate operability risks:

Further evaluation of LDI concepts were performed and designs were selected for hydrogen combustion laboratory testing at GRC.

Premixed swirler designs were evaluated and the most promising one was selected for CFD modeling. To validate CFD, a model of a similar swirler was run and compared with experimental results. So far, CFD accuracy in modeling species profiles and hence mixing for this swirler has proven poor. Further model development is being done to improve accuracy.

Efforts to further validate CFD NOx and H2 combustion models showed a significant difference in NOx depending on choice of software, combustion model, and NOx model. As experimental results from the GRC LDI tests become available, the models will be further developed to improve accuracy.

References [Results and Discussion Section]

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- 3. A. R. Choudhuri, S. R. Gollahalli, Journal of Propulsion and Power, Vol. 19, No. 2, 2003.

List of Acronyms and Abbreviations

CFD Computational Fluid Dynamics

CRM Chemical Network Model

DACR Dual Annular Counter Rotating

DLN Dry Low NOx

DOE Design of Experiments

FMEA Failure Mode Effects Analysis

GE General Electric Company

GRC GE Global Research Center

IGCC Integrated Gasification Combined Cycle

LDI Lean Direct Injection

MVT Multi Venturi Tube

MPLDI Multiple Point Lean Direct Injection

PFR Plug Flow Reactor

PLC Programmable Logic Controller

PLIF Planar Laser Induced Fluorescence

PSR Perfectly Stirred Reactor

QFD Quality Function Deployment

RAM Reliability and Maintainability